Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America

NEWS 2 "Ask CAS" for self-help around the clock

NEWS 3 JUL 20 Powerful new interactive analysis and visualization software, STN AnaVist, now available

NEWS 4 AUG 11 Derwent World Patents Index(R) web-based training during August

NEWS 5 AUG 11 STN AnaVist workshops to be held in North America

NEWS 6 AUG 30 CA/CAplus -Increased access to 19th century research documents

NEWS 7 AUG 30 CASREACT - Enhanced with displayable reaction conditions

NEWS 8 SEP 09 ACD predicted properties enhanced in REGISTRY/ZREGISTRY

NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS INTER General Internet Information

NEWS LOGIN Welcome Banner and News Items

NEWS PHONE Direct Dial and Telecommunication Network Access to STN

NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 11:53:29 ON 21 SEP 2005

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

0.21 0.21

FULL ESTIMATED COST

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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

```
=> e 1,3-indandicarboxylic acid/cn
                   1,3-INDANDIAMINE/CN
E1
             1
                   1,3-INDANDIAMINE, 2-PHENYL-, DIHYDROCHLORIDE/CN
E2
             1
             0 --> 1,3-INDANDICARBOXYLIC ACID/CN
E3
                   1,3-INDANDICARBOXYLIC ACID ANHYDRIDE/CN
E4
             1
                   1,3-INDANDIOL/CN
E5
             1
                   1,3-INDANDIOL, 1,2,2,3-TETRAPHENYL-/CN
E6
             1
                   1,3-INDANDIOL, 1,2,3-TRIBENZYL-/CN
E7
             1
                   1,3-INDANDIOL, 1,2,3-TRIPHENYL-2-(2-PIPERIDYL)-/CN
E8
             1
                   1,3-INDANDIOL, 1,2,3-TRIPHENYL-2-(2-PYRIDYL)-/CN
E9
             1
                   1,3-INDANDIOL, 1,3-DI-1-NAPHTHYL-2-(PHENYLAZO)-/CN
E10
             1
                   1,3-INDANDIOL, 1,3-DI-P-TOLYL-2-(M-TOLYLAZO)-/CN
E11
             1
                   1,3-INDANDIOL, 1,3-DI-P-TOLYL-2-(O-TOLYLAZO)-/CN
E12
             1
=> e indan-1,3-dicarboxylic acid/cn
                   INDAN-1,2,3-TRIONE 2-(N-BENZOYL-N-PHENYLHYDRAZONE) COMPD. WI
E1
                   TH INDAN-1,2,3-TRIONE 2-(N-PHENYLHYDRAZONE) (1:1)/CN
                   INDAN-1,2,3-TRIONE 2-(N-P-TERT-BUTYLBENZOYL-N-PHENYLHYDRAZON
E2
             1
                   E)/CN
             0 --> INDAN-1,3-DICARBOXYLIC ACID/CN
E3
                   INDAN-1,3-DIONE ANION/CN
E4
             1
                   INDAN-1,3-DIONE, 2-(1-OXOINDEN-2-YL)-/CN
E5
             1
                   INDAN-1-ACETYL CHLORIDE/CN
             1
E6
                   INDAN-1-ONE N, N-DIMETHYLHYDRAZONE/CN
E7
             1
                   INDAN-1-ONE-6-CARBOXYLIC ACID/CN
             1
E8
                   INDAN-1-YL METHYL ETHER/CN
E9
             1
                   INDAN-1-YLTHIOACETIC ACID S-(PYRIDIN-2-YL) ESTER/CN
E10
             1
                   INDAN-2,2-DIPHOSPHONIC ACID/CN
E11
             1
                   INDAN-2-14C/CN
E12
             1
```

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10706694\10706694 product.str

chain nodes : 10 11

ring nodes :

 $1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad 8 \quad 9$ 

chain bonds : 7-10 9-11 ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds: 5-7 6-9 7-8 8-9 exact bonds: 7-10 9-11

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS

# L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam
SAMPLE SEARCH INITIATED 11:58:04 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2019 TO ITERATE

99.1% PROCESSED 2000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

37685 TO 43075

PROJECTED ANSWERS:

0 TO 0

L2

L3

0 SEA SSS SAM L1

=> search l1 sss full

FULL SEARCH INITIATED 11:58:26 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 41894 TO ITERATE

100.0% PROCESSED 41894 ITERATIONS

8 ANSWERS

0 ANSWERS

SEARCH TIME: 00.00.01

8 SEA SSS FUL L1

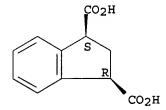
=> d scan

L3 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1H-Indene-1,3-dicarboxylic acid, 2,3-dihydro-, cis- (9CI)

MF C11 H10 O4

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):8

L3 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1H-Indene-1,3-dicarboxylic acid, 1-amino-2,3-dihydro-, (1R,3S)-rel- (9CI)

MF C11 H11 N O4

Relative stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 1H-Indene-1,3-dicarboxylic acid, 1-amino-2,3-dihydro-, (1R,3R)-rel- (9CI)
MF C11 H11 N O4

Relative stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN 1H-Indene-1,3-dicarboxylic acid, 2,3-dihydro- (9CI) MF C11 H10 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 1H-Indene-1,3-dicarboxylic acid, 1-amino-2,3-dihydro-, (1R,3S)- (9CI)
MF C11 H11 N O4

Absolute stereochemistry. Rotation (-).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 1H-Indene-1,3-dicarboxylic acid, 1-amino-2,3-dihydro-, (1R,3R)- (9CI)
MF C11 H11 N O4

Absolute stereochemistry. Rotation (-).

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1,2,3-Indantricarboxylic acid, 1-(carboxymethyl)- (5CI)

MF C14 H12 O8

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1H-Indene-1,3-dicarboxylic acid, 4,5,6,7-tetrafluoro-2,3-dihydro- (9CI)

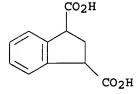
MF C11 H6 F4 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

## ALL ANSWERS HAVE BEEN SCANNED

```
=> e 1H-Indene-1,3-dicarboxylic acid, 2,3-dihydro-/cn
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 1-BENZOYL-2-PHENYL-, DIMETH
E1
             1
                   YL ESTER/CN
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 1-BUTYL-, DIBUTYL ESTER/CN
E2
             1
E3
             1 --> 1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-/CN
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-, CIS-/CN
E4
             1
E5
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-1-((METHOXYCARB
             1
```

```
ONYL) AMINO) -, DIMETHYL ESTER, (1R, 3R) -/CN
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-1-((METHOXYCARB
E6
             1
                   ONYL) AMINO) -, DIMETHYL ESTER, (1R, 3S) -/CN
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 2-PHENYL-/CN
E7
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 2-PHENYL-, DIMETHYL ESTER/C
E8
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 2-PHENYL-, POLYMER WITH 1,1
E9
             1
                   '-OXYBIS (4-ISOCYANATOBENZENE)/CN
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 2-PHENYL-, POLYMER WITH 1,4
             1
E10
                   -BENZENEDICARBOXYLIC ACID AND 1,1'-OXYBIS(4-ISOCYANATOBENZEN
                   E)/CN
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 4,5,6,7-TETRAFLUORO-2,3-DIH
             1
E11
                   YDRO-/CN
             1
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 4-(ACETYLOXY)OCTAHYDRO-3A-M
E12
                   ETHYL-6-(1-METHYLETHYL)-7-OXO-/CN
=> e3
             1 "1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-"/CN
L4
=> d 14
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
1.4
     343317-37-3 REGISTRY
RN
     Entered STN: 26 Jun 2001
ED
     1H-Indene-1,3-dicarboxylic acid, 2,3-dihydro- (9CI) (CA INDEX
CN
     NAME)
FS
     3D CONCORD
     C11 H10 O4
MF
     Reaction Database
SR
     STN Files: CA, CAPLUS, CASREACT
LC
```



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
171.64
171.85

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FILE COVERS 1907 - 21 Sep 2005 VOL 143 ISS 13 FILE LAST UPDATED: 20 Sep 2005 (20050920/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=>14L5 1 L4 => d l5 ti fbib abs ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN 1.5 A method for preparing indan-1,3-dicarboxylic acid TΤ AN 2004:453158 CAPLUS

DN 141:23306 A method for preparing indan-1,3-dicarboxylic acid TI

Arpin, Patric; Guzman, Mark Christopher; Watson, Timothy James Norman IN

Pfizer Products Inc., USA PA

PCT Int. Appl., 13 pp. so CODEN: PIXXD2

DTPatent

English LA

FAN.CNT 1

```
KIND
                               DATE
                                          APPLICATION NO.
                                                                  DATE
     PATENT NO.
                         ____
                                                                   _____
     WO 2004046077
                                           WO 2003-IB5043
                                                                   20031107
PΙ
                         A1
                                20040603
                         C1
                                20050519
     WO 2004046077
           AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
             TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
            BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,
                                            US 2002-427981P
                                                             P 20021120
     CA 2502443
                                20040603
                                            CA 2003-2502443
                                                                   20031107
                         ΔΔ
                                            US 2002-427981P
                                                                P 20021120
                                            WO 2003-IB5043
                                                                W 20031107
     EP 1565421
                                20050824
                                            EP 2003-758601
                                                                   20031107
                         A1
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
                                                                P 20021120
                                            US 2002-427981P
                                            WO 2003-IB5043
                                                                W 20031107
```

CASREACT 141:23306; MARPAT 141:23306 OS

A method for preparing indan-1,3-dicarboxylic acid (I) and its AB ring-substituted derivs. comprises the cyclocondensation reaction of an 2-(2-halophenyl)acetonitrile with 3-ethoxyacrylonitrile in the presence of palladium diacetate, tricyclohexylphosphine, and a base in a water-miscible organic solvent to give 1,3-indenedinitrile which is then hydrogenated into indan-1,3-dinitrile and hydrolyzed into I.

```
=> filoe reg
             0 FILOE
          1148 REG
            60 REGS
```

## 1202 REG

(REG OR REGS)
O FILOE REG

L6

(FILOE(W) REG)

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	7.33	179.18
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.73	-0.73

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STRUCTURE FILE UPDATES: 19 SEP 2005 HIGHEST RN 863478-08-4 DICTIONARY FILE UPDATES: 19 SEP 2005 HIGHEST RN 863478-08-4

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Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

## => e 1,3-indenedinitrile/cn

E1	1	1,3-INDANEDIONE, 2-(P-(DIETHYLAMINO)PHENYL)-2-(2-PIPERIDINOE
		THYL)-, DIHYDROBROMIDE/CN
E2	1	1,3-INDENEDICARBOXYLIC ACID/CN
E3	0>	1,3-INDENEDINITRILE/CN
E4	1	1,3-INDENEDIOL, 1-METHYL-/CN
E5	1	1,3-INDOLEDIACETIC ACID, A,A,A',A'-T
		ETRAMETHYL-/CN
E6	1	1,3-INDOLEDIACETIC ACID, 2-CARBOXY-, DIETHYL ESTER/CN
E7	1	1,3-INDOLEDIOL, 5-METHOXY-6-NITRO-2-PHENYL-, DIACETATE/CN
E8	1	1,3-INDOLEDIPROPIONITRILE, 2-PHENYL-/CN
E9	1	1,3-INDOLINEDIPROPIONIC ACID, 2-OXO-/CN
E10	1	1,3-INDOLIZINEDIACETIC ACID, A,A'-DIHYDROXY-2-PH
		ENYL-A, A'-BIS (TRIFLUOROMETHYL)-, DIMETHYL ESTER/
		CN
E11	1	1,3-INDOLIZINEDIACETIC ACID, 2,5-DIMETHYL-A,A'-D

E12

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 0.86 180.04

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

CA SUBSCRIBER PRICE ENTRY SESSION 0.00 -0.73

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FILE COVERS 1907 - 21 Sep 2005 VOL 143 ISS 13 FILE LAST UPDATED: 20 Sep 2005 (20050920/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 11:53:29 ON 21 SEP 2005)

FILE 'REGISTRY' ENTERED AT 11:53:57 ON 21 SEP 2005

E 1,3-INDANDICARBOXYLIC ACID/CN

E INDAN-1,3-DICARBOXYLIC ACID/CN

L1 STRUCTURE UPLOADED

L2 0 SEARCH L1 SSS SAM

L3 8 SEARCH L1 SSS FULL

E 1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-/CN

L4 1 E3

FILE 'CAPLUS' ENTERED AT 12:00:12 ON 21 SEP 2005

L5 1 L4

L6 0 FILOE REG

FILE 'REGISTRY' ENTERED AT 12:01:07 ON 21 SEP 2005 E 1,3-INDENEDINITRILE/CN

FILE 'CAPLUS' ENTERED AT 12:02:18 ON 21 SEP 2005

=> 13

L7 6 L3

=> ?nitrile

L8 327361 ?NITRILE

=> 17 and 18

```
=> d 19
```

```
ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
L9
AN
     2004:453158 CAPLUS
     141:23306
DN
     A method for preparing indan-1,3-dicarboxylic acid
TΙ
     Arpin, Patric; Guzman, Mark Christopher; Watson, Timothy James Norman
IN
     Pfizer Products Inc., USA
PA
     PCT Int. Appl., 13 pp.
so
     CODEN: PIXXD2
DT
     Patent
LA
    English
FAN.CNT 1
     PATENT NO.
                        KIND
                                DATE
                                          APPLICATION NO.
                                                                   DATE
                         _ _ _ _
                                -----
                                            -----
                                                                   -----
PΙ
    WO 2004046077
                         A 1
                                20040603
                                           WO 2003-IB5043
                                                                   20031107
                                20050519
     WO 2004046077
                         C1
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
            LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
             TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
            BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2502443
                         AA
                                20040603
                                         CA 2003-2502443
                                                                   20031107
     EP 1565421
                          A1
                                20050824
                                          EP 2003-758601
                                                                   20031107
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
PRAI US 2002-427981P
                        P
                                20021120
    WO 2003-IB5043
                         W
                                20031107
     CASREACT 141:23306; MARPAT 141:23306
OS
=> logoff hold
                                                 SINCE FILE
COST IN U.S. DOLLARS
                                                                 TOTAL
                                                      ENTRY
                                                               SESSION
FULL ESTIMATED COST
                                                       5.69
                                                                185.73
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                                 SINCE FILE
                                                                 TOTAL
                                                      ENTRY
                                                               SESSION
                                                       0.00
                                                                 -0.73
CA SUBSCRIBER PRICE
 SESSION WILL BE HELD FOR 60 MINUTES
```

STN INTERNATIONAL SESSION SUSPENDED AT 12:06:01 ON 21 SEP 2005

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

#### PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \* SESSION RESUMED IN FILE 'CAPLUS' AT 12:08:47 ON 21 SEP 2005 FILE 'CAPLUS' ENTERED AT 12:08:47 ON 21 SEP 2005 COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

SINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION 5.69 185.73 FULL ESTIMATED COST SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) ENTRY SESSION 0.00 -0.73 CA SUBSCRIBER PRICE => d his (FILE 'HOME' ENTERED AT 11:53:29 ON 21 SEP 2005) FILE 'REGISTRY' ENTERED AT 11:53:57 ON 21 SEP 2005 E 1,3-INDANDICARBOXYLIC ACID/CN E INDAN-1,3-DICARBOXYLIC ACID/CN STRUCTURE UPLOADED L1 0 SEARCH L1 SSS SAM L2 L3 8 SEARCH L1 SSS FULL E 1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-/CN T.4 FILE 'CAPLUS' ENTERED AT 12:00:12 ON 21 SEP 2005 L5 1 L4 0 FILOE REG L6 FILE 'REGISTRY' ENTERED AT 12:01:07 ON 21 SEP 2005 E 1,3-INDENEDINITRILE/CN FILE 'CAPLUS' ENTERED AT 12:02:18 ON 21 SEP 2005 L7 6 L3 327361 ?NITRILE L8 L9 1 L7 AND L8 => save temp 17 indanefinds/a ANSWER SET L7 HAS BEEN SAVED AS 'INDANEFINDS/A' => save temp all indansrch/l L# LIST L1-L9 HAS BEEN SAVED AS 'INDANSRCH/L' => cyano 77597 CYANO 3 CYANOS L10 77598 CYANO (CYANO OR CYANOS) => 17 and 110 0 L7 AND L10 L11 => logoff hold SINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION FULL ESTIMATED COST 9.83 189.87 SINCE FILE DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) TOTAL ENTRY SESSION 0.00 -0.73 CA SUBSCRIBER PRICE SESSION WILL BE HELD FOR 60 MINUTES STN INTERNATIONAL SESSION SUSPENDED AT 12:11:33 ON 21 SEP 2005

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \* \* SESSION RESUMED IN FILE 'CAPLUS' AT 12:47:46 ON 21 SEP 2005 FILE 'CAPLUS' ENTERED AT 12:47:46 ON 21 SEP 2005

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COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
9.83
189.87

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY

CA SUBSCRIBER PRICE

0.00

-0.73

=> d his

(FILE 'HOME' ENTERED AT 11:53:29 ON 21 SEP 2005)

FILE 'REGISTRY' ENTERED AT 11:53:57 ON 21 SEP 2005

E 1,3-INDANDICARBOXYLIC ACID/CN
E INDAN-1,3-DICARBOXYLIC ACID/CN

L1 STRUCTURE UPLOADED L2 0 SEARCH L1 SSS SAM

L3 8 SEARCH L1 SSS FULL

E 1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-/CN

L4 1 E3

FILE 'CAPLUS' ENTERED AT 12:00:12 ON 21 SEP 2005

L5 1 L4

L6 0 FILOE REG

FILE 'REGISTRY' ENTERED AT 12:01:07 ON 21 SEP 2005 E 1.3-INDENEDINITRILE/CN

FILE 'CAPLUS' ENTERED AT 12:02:18 ON 21 SEP 2005

L7 6 L3

L8 327361 ?NITRILE L9 1 L7 AND L8

> SAVE TEMP L7 INDANEFINDS/A SAVE TEMP ALL INDANSRCH/L

L10 77598 CYANO

L11 0 L7 AND L10

=> logoff hold

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
SINCE FILE
TOTAL

CA SUBSCRIBER PRICE 101AL ENTRY SESSION 0.00 -0.73

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 12:48:18 ON 21 SEP 2005

Connecting via Winsock to STN

#### LOGINID: SSSPTA1623PAZ

## PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \* \* SESSION RESUMED IN FILE 'CAPLUS' AT 13:32:07 ON 21 SEP 2005 FILE 'CAPLUS' ENTERED AT 13:32:07 ON 21 SEP 2005 COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
10.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

ENTRY
SESSION
CA SUBSCRIBER PRICE

0.00
-0.73

=> logofff hold

0 LOGOFFF 35891 HOLD 24794 HOLDS 59782 HOLD

(HOLD OR HOLDS)
0 LOGOFFF HOLD

L12

(LOGOFFF(W)HOLD)

#### => ind?n?

'?' TRUNCATION SYMBOL NOT VALID WITHIN 'IND?N?'
The truncation symbol? may be used only at the end of a search
term. To specify a variable character within a word use '!', e.g.,
'wom!n' to search for both 'woman' and 'women'. Enter "HELP
TRUNCATION" at an arrow prompt (=>) for more information.

## => ind?ne

'?' TRUNCATION SYMBOL NOT VALID WITHIN 'IND?NE'
The truncation symbol? may be used only at the end of a search
term. To specify a variable character within a word use '!', e.g.,
'wom!n' to search for both 'woman' and 'women'. Enter "HELP
TRUNCATION" at an arrow prompt (=>) for more information.

=> file reg

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
16.31
196.35

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION
CA SUBSCRIBER PRICE

0.00
-0.73

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 SEP 2005 HIGHEST RN 863478-08-4 DICTIONARY FILE UPDATES: 19 SEP 2005 HIGHEST RN 863478-08-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

\* The CA roles and document type information have been removed from \*

\* the IDE default display format and the ED field has been added, \*

\* effective March 20, 2005. A new display format, IDERL, is now \*

\* available and contains the CA role and document type information. \*

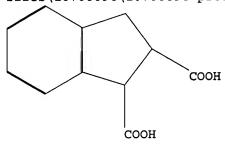
\*

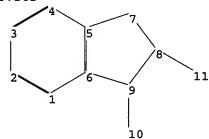
Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10706694\10706694 product isomer.str





chain nodes :

10 11

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds : 8-11 9-10 ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds: 5-7 6-9 7-8 8-9 exact bonds: 8-11 9-10

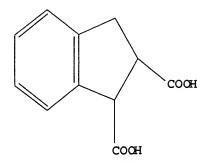
normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS

L13 STRUCTURE UPLOADED

=> d 113 L13 HAS NO ANSWERS L13 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 113 sss sam

SAMPLE SEARCH INITIATED 13:35:18 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 498 TO ITERATE

100.0% PROCESSED 498 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

8622 TO 11298

PROJECTED ANSWERS:

1 TO 8

L14

1 SEA SSS SAM L13

=> d scan

L14 1 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1,2-Indandicarboxylic acid, 5,6,7-trimethoxy- (5CI)

MF C14 H16 O7

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

## ALL ANSWERS HAVE BEEN SCANNED

```
=> e 1,2-Indandicarboxylic acid/cn
                   1,2-INDANDICARBOXIMIDE, N-POTASSIUM DERIV/CN
E1
                   1,2-INDANDICARBOXIMIDE, N-PROPYL-/CN
E2
              --> 1,2-INDANDICARBOXYLIC ACID/CN
E3
             0
                   1,2-INDANDICARBOXYLIC ACID, 2-(CARBOXYMETHYL)-7-METHYL-3-OXO
E4
                   -, TRIMETHYL ESTER/CN
                   1,2-INDANDICARBOXYLIC ACID, 2-HYDROXY-/CN
             1
E5
                   1,2-INDANDICARBOXYLIC ACID, 3-((CARBOXYAMINO)METHYL)-, TRIME
E6
             1
                   THYL ESTER/CN
                   1,2-INDANDICARBOXYLIC ACID, 3-HYDROXY-6-METHOXY-, DIMETHYL E
             1
E7
                   STER/CN
```

```
1,2-INDANDICARBOXYLIC ACID, 4,5,6,7-TETRAMETHYL-/CN
E8
                   1,2-INDANDICARBOXYLIC ACID, 4,5,6,7-TETRAMETHYL-, DIMETHYL E
E9
             1
                   STER/CN
                   1,2-INDANDICARBOXYLIC ACID, 5,6,7-TRIMETHOXY-/CN
E10
             1
                   1,2-INDANDICARBOXYLIC ACID, 5,6,7-TRIMETHOXY-, DIETHYL ESTER
E11
             1
                   /CN
                   1,2-INDANDICARBOXYLIC ACID, 5,6-DIMETHOXY-, DIETHYL ESTER/CN
E12
             1
=> file caplus
                                                  SINCE FILE
                                                                   TOTAL
COST IN U.S. DOLLARS
                                                       ENTRY
                                                                 SESSION
                                                        2.15
                                                                 198.50
FULL ESTIMATED COST
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                                  SINCE FILE
                                                                   TOTAL
                                                       ENTRY
                                                                 SESSION
                                                        0.00
                                                                   -0.73
CA SUBSCRIBER PRICE
```

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FILE COVERS 1907 - 21 Sep 2005 VOL 143 ISS 13 FILE LAST UPDATED: 20 Sep 2005 (20050920/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 1,2-Indandicarboxylic
8400853 1
8498306 2
113 INDANDICARBOXYLIC
L15 20 1,2-INDANDICARBOXYLIC
(1(W)2(W)INDANDICARBOXYLIC)

=> d hsi
'HSI' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ------ GI and AB
ALL ------ BIB, AB, IND, RE
APPS ------ AI, PRAI
BIB ------ AN, plus Bibliographic Data and PI table (default)
CAN ------ List of CA abstract numbers without answer numbers
CBIB ------ AN, plus Compressed Bibliographic Data
DALL ------ ALL, delimited (end of each field identified)
DMAX ------ MAX, delimited for post-processing
FAM ------ AN, PI and PRAI in table, plus Patent Family data
FBIB ------ AN, BIB, plus Patent FAM
IND ------ Indexing data
IPC ------ International Patent Classifications

```
MAX ----- ALL, plus Patent FAM, RE
PATS ----- PI, SO
SAM ----- CC, SX, TI, ST, IT
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
             SCAN must be entered on the same line as the DISPLAY,
             e.g., D SCAN or DISPLAY SCAN)
STD ----- BIB, IPC, and NCL
IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IMAX ----- MAX, indented with text labels
ISTD ----- STD, indented with text labels
OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels
SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations
HIT ----- Fields containing hit terms
HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
             containing hit terms
HITRN ----- HIT RN and its text modification
HITSTR ----- HIT RN, its text modification, its CA index name, and
             its structure diagram
HITSEQ ----- HIT RN, its text modification, its CA index name, its
             structure diagram, plus NTE and SEQ fields
FHITSTR ---- First HIT RN, its text modification, its CA index name, and
             its structure diagram
FHITSEQ ---- First HIT RN, its text modification, its CA index name, its
             structure diagram, plus NTE and SEQ fields
KWIC ----- Hit term plus 20 words on either side
OCC ----- Number of occurrence of hit term and field in which it occurs
To display a particular field or fields, enter the display field
codes. For a list of the display field codes, enter HELP DFIELDS at
an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST;
TI, IND; TI, SO. You may specify the format fields in any order and the
information will be displayed in the same order as the format
specification.
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FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC
to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):\end
'\END' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'
The following are valid formats:
ABS ----- GI and AB
ALL ----- BIB, AB, IND, RE
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data and PI table (default)
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
DALL ----- ALL, delimited (end of each field identified)
DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data
IPC ----- International Patent Classifications
MAX ----- ALL, plus Patent FAM, RE
PATS ----- PI, SO
SAM ----- CC, SX, TI, ST, IT
```

SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers; SCAN must be entered on the same line as the DISPLAY, e.g., D SCAN or DISPLAY SCAN) STD ----- BIB, IPC, and NCL IABS ----- ABS, indented with text labels IALL ----- ALL, indented with text labels IBIB ----- BIB, indented with text labels IMAX ----- MAX, indented with text labels ISTD ----- STD, indented with text labels OBIB ----- AN, plus Bibliographic Data (original) OIBIB ----- OBIB, indented with text labels SBIB ----- BIB, no citations SIBIB ----- IBIB, no citations HIT ----- Fields containing hit terms HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT) containing hit terms HITRN ----- HIT RN and its text modification HITSTR ----- HIT RN, its text modification, its CA index name, and its structure diagram HITSEQ ----- HIT RN, its text modification, its CA index name, its structure diagram, plus NTE and SEQ fields FHITSTR ---- First HIT RN, its text modification, its CA index name, and its structure diagram FHITSEQ ---- First HIT RN, its text modification, its CA index name, its structure diagram, plus NTE and SEQ fields KWIC ----- Hit term plus 20 words on either side OCC ----- Number of occurrence of hit term and field in which it occurs To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI, IND; TI, SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification. All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number. ENTER DISPLAY FORMAT (BIB) : end => d his (FILE 'HOME' ENTERED AT 11:53:29 ON 21 SEP 2005) FILE 'REGISTRY' ENTERED AT 11:53:57 ON 21 SEP 2005 E 1,3-INDANDICARBOXYLIC ACID/CN E INDAN-1, 3-DICARBOXYLIC ACID/CN STRUCTURE UPLOADED L1 0 SEARCH L1 SSS SAM L2 8 SEARCH L1 SSS FULL L3 E 1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-/CN L41 E3 FILE 'CAPLUS' ENTERED AT 12:00:12 ON 21 SEP 2005 1 L4 L5 O FILOE REG **L6** FILE 'REGISTRY' ENTERED AT 12:01:07 ON 21 SEP 2005

FILE 'CAPLUS' ENTERED AT 12:02:18 ON 21 SEP 2005

E 1,3-INDENEDINITRILE/CN

```
L7
              6 L3
L8
         327361 ?NITRILE
L9
              1 L7 AND L8
                SAVE TEMP L7 INDANEFINDS/A
                SAVE TEMP ALL INDANSRCH/L
L10
          77598 CYANO
              0 L7 AND L10
L11
L12
              0 LOGOFFF HOLD
     FILE 'REGISTRY' ENTERED AT 13:34:53 ON 21 SEP 2005
L13
                STRUCTURE UPLOADED
              1 SEARCH L13 SSS SAM
L14
                E 1,2-INDANDICARBOXYLIC ACID/CN
     FILE 'CAPLUS' ENTERED AT 13:38:00 ON 21 SEP 2005
             20 1,2-INDANDICARBOXYLIC
L15
=> 18 and 115
             2 L8 AND L15
L16
=> d l16 ti fbib abs
    ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
     Synthesis of compounds related to gibberellic acid. II. (±)-Gibberic
TI
     acid
AN
     1965:51435 CAPLUS
     62:51435
DN
OREF 62:9079f-g
     Synthesis of compounds related to gibberellic acid. II. (\pm)-Gibberic
ΤI
ΙΙΔ
     Loewenthal, H. J. E.; Malhotra, S. K.
     Israel Inst. Technol. Haifa
CS
     Journal of the Chemical Society, Abstracts (1965), (Feb.), 990-4
SO
     CODEN: JCSAAZ; ISSN: 0590-9791
DT
     Journal
     English
LA
     CASREACT 62:51435
OS
     For diagram(s), see printed CA Issue.
GI
     (t)-Gibberic acid (I), a key degradation product of gibberellic acid,
AB
     was synthesized from o- tolylacetonitrile. Cf CA 58,
     10140a.
=> d 116 2 ti fbib abs
    ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
L16
     Synthesis of cis-8-methylhydrindanone
TΙ
AN
     1958:35125 CAPLUS
     52:35125
DN
OREF 52:6294i,6295a-i
     Synthesis of cis-8-methylhydrindanone
TI
     Chatterjee, Ramesh Chandra; Bhattacharyya, Bidyut Kamal
ΑU
     Jadavpur Univ., Calcutta
CS
     J. Indian Chem. Soc. (1957), 34, 515-27
SO
DT
     Journal
     Unavailable
LA
     cf. C.A. 51, 331h. NCCH2CO2Et (115 ml.), 115 g. Et 2-methylcyclohexanone-
AB
     2-carboxylate, 30 ml. AcOH, and 12 g. AcONH4 in 250 ml. C6H6 was refluxed
     with continuous removal of H2O; an addnl. 48 g. AcONH4 was added in 12 g.
     lots as the reaction slowed. After 30 hrs. refluxing, the mixture on
     cooling deposited 15 g. 2-methyl-2-carboxycyclohexylidene-1-cyanoacetic
     acid imide, m. 230-1° (EtOH), \lambda 220 m\mu (log \epsilon
     4.026) (alc.); after removal of this byproduct, the main product was
     worked up by distillation to give 107 g. Et
```

2-methyl-2-carbethoxycyclohexylidene-

1-cyanoacetate (I), b1 165-8°, n25D 1.4762; acid (HCl hydrolysis of I), m. 169-70°, also obtainable by the alkali hydrolysis of the above imide. To 5.75 g. Na in 200 ml. absolute EtOH at 0-5° 70 g. I was introduced dropwise, after 1 hr. 48 g. BrCH2CO2Et added followed by refluxing 16 hrs.; working up yielded 77 g. di-Et  $\alpha$ -cyano- $\alpha$ -(2methyl-2-carbethoxy-6-cyclohexenyl) succinate (II), b1 195-200°, n25D 1.4780. II (58 g.) refluxed 36 hrs. with 650 ml. concentrated HCl, most the HCl distilled, and the product worked up with Et2O and crystallized from Et20 and petr. ether (40-60°) gave 8 g. mixture of acids, m. 130-45°; crystallization from 25 ml. AcOEt, 200 ml. Et2O, and 50 ml. petr. ether gave 3.2 g. 2-methyl-2-carboxycyclohex-6-enylsuccinic acid lactone (III), m. 184-5° (Et2O-petr. ether); working up the mother liquors gave 6.8 g. 2-methyl-2-carboxycyclohex-6-enylsuccinic acid (IV), m. 152-3° (ether-petr. ether). When the time of hydrolysis was increased to 55 hrs., 4.6 g. 2-methyl-1-cyclohexenylsuccinic acid lactone (V), m. 200° (Et20-petr. ether) (Me ester, b0.8 140-5°), along with a gummy acid mixture was obtained. The crude acid mixture was esterified with MeOH and H2SO4 50 hrs., and the Et2OC6H6 extract separated into neutral and acid parts with 5% aqueous NaOH. Distillation of the neutral part gave 29.5 g. Me ester (VI) of IV, b0.8 155-60°, n26D 1.4819, and the alkaline portion was worked up to yield 1.8 g. Me ester of III, b0.5 160-9°. IV (1 g.) and 20 ml. concentrated HCl was refluxed 20 hrs. to give 0.1 g. III; when heated for a much longer time only 13 mg. V could be isolated. When 10.3 g. VI in 40 ml. C6H6 was cyclized with MeONa (from 1.57 g. Na, 2.8 ml. MeOH, and 30 ml. C6H6) at reflux temperature 4-5 hrs. under N, 5.3 g. di-Me  $\Delta$ 3a,4-7a-methylhydrindanone-2,3-dicarboxylate (VII), b1.5 165-8°, n25D 1.4935, λ 220 mμ (alc.) (log ε 3.81), was obtained; with Na dust alone the yield was only 2.8 g. VII (20.5 g.) was refluxed 32 hrs. with 100 ml. concentrated HCl and worked up with Et20 to give 0.28 g. neutral ketone (VIII) and 10.2 g. Δ3a,4-3-carboxy-7a-methylhydrindanone (IX), m. 160° (Et20-petr. ether) (semicarbazone, m. 258°); Me ester, b1.5 120-5° [semicarbazone, m. 220° (dilute MeOH)]. III (1.15 g.) in 5 ml. MeOH was refluxed with 0.23 g. Na in 5 ml. MeOH 2 hrs., cooled, treated with 5 ml. MeI, and refluxed 6 hrs. to give 0.83 g. VI. VI (8 g.) in AcOH was hydrogenated over prereduced PtO2 to give 7.8 g. dihydro derivative (X), b1 155-7°, n33D 1.4715. X (7.8 g.) on cyclization with MeONa in C6H6 gave 4 g. cis-dimethyl-7a-methylhydrindanone-2,3dicarboxylate (XI), b0.5 135-40°. Hydrogenation of IX in AcOH over prereduced PtO2 yielded cis-7a-methylhydrindanone-3-carboxylic acid (XII), m. 155-6°; Me ester, b0.9 120° (semicarbazone, m. 192-3°). Acid hydrolysis of XI gave XII which (1.38 g.) on oxidation with HNO3 gave cis-2-methylcyclohexane-1,2-dicarboxylic acid, m. 160°. Hydrogenation of VIII gave cis-7a-methylhydrindanone (XIII),

isolated as the semicarbazone, m. 223° (dilute MeOH). IX (0.8 g.) was decarboxylated in 5 ml. quinoline at 250-70° in the presence of Cu and the resulting product hydrogenated over 10% Pd-C to give XIII. Condensation of 11.2 g. 2-methylcyclohexanone with di-Me succinate in the

125-7°; dihydro di-Me ester (XIV), b4 125-6°. Saponification of XIV with 10% MeOH-NaOH yielded  $\alpha$ -(2-methylcyclohexyl) succinic acid (XV), m. 155°. V (0.424 g.) in 14 ml. MeOH was refluxed with MeONa 2

0.45 g. HO ester (XVI), b0.2-0.3 110-12°. Dehydration of XVI with

hrs., cooled, and refluxed 6 hrs. after the addition of 2 ml. MeI to give

(2-methylcyclohexylidene) cyanoacetate with 17 g. BrCH2CO2Et, gave 17.6 g.

presence of tert-BuOK gave 15.8 g.  $\beta$ -carbomethoxy- $\beta$ -(o-

KHSO4 at 180° under N gave the unsatd. diester, b0.2 90-100°; dihydro derivative (XVII), b0.4 110-15°. Acid hydrolysis of XVII gave XV. Condensation of 19.4 g. Et

methylcyclohexenyl) propionic acid, b0.5 145-50°; Me ester, b4

di-Et  $\alpha$ -cyano- $\alpha$ -(2-methylcyclohexenyl) succinate (XVIII), b1 168-75°, n25D 1.4740. XVIII (6.8 g.) was heated with 125 ml. concentrated HCl 16 hrs. to give 2.1 g.  $\gamma$ -(2-methylcyclohexyl)- $\beta$ -

of

carboxyspirobutyrolactone (XIX), m. 107° (Et20-petr. ether). XIX (2.55 g.) on decarboxylation at 240-50° in the presence of powdered glass gave 1.6 g.  $\gamma$ -(2-methylcyclohexyl)spirobutyrolactone, b4 130-5°.

=> save temp all indansrch/l

'INDANSRCH/L' IN USE

A single name cannot be used for two saved items at the same time. Enter "Y" if you wish to replace the current saved name with a new definition. Enter "N" if the current saved definition must be preserved. You may then reenter the SAVE command with a different saved name. Enter "DISPLAY SAVED" at an arrow prompt (=>) to see a list of your currently defined saved names.

REPLACE OLD DEFINITION? Y/(N):y

L# LIST L1-L16 HAS BEEN SAVED AS 'INDANSRCH/L'

=> logoff hold

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 17.27 215.77 SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SESSION ENTRY -2.19 -1.46 CA SUBSCRIBER PRICE

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STN INTERNATIONAL SESSION SUSPENDED AT 13:46:18 ON 21 SEP 2005

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS 6 AUG 30 CA/CAplus -Increased access to 19th century research documents

NEWS 7 AUG 30 CASREACT - Enhanced with displayable reaction conditions

NEWS 8 SEP 09 ACD predicted properties enhanced in REGISTRY/ZREGISTRY

NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

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=> file regh
'REGH' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'HOME'

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> file reg COST IN U.S. DOLLARS

Marian san a caledar

SINCE FILE TOTAL ENTRY SESSION 0.42 0.42

FULL ESTIMATED COST

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 SEP 2005 HIGHEST RN 863636-50-4 DICTIONARY FILE UPDATES: 21 SEP 2005 HIGHEST RN 863636-50-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

```
=> e 1H-Indene-1,3-dicarboxylic acid, 2,3-dihydro-, cis-/cn
E1 1 1H-INDENE-1,3-DICARBOXYLIC ACID, 1-BUTYL-, DIBUTYL ESTER/CN
E2 1 1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-/CN
E3 1 --> 1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-, CIS-/CN
```

```
1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-1-((METHOXYCARB
E4
             1
                   ONYL) AMINO) -, DIMETHYL ESTER, (1R, 3R) -/CN
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-1-((METHOXYCARB
E5
             1
                   ONYL) AMINO) -, DIMETHYL ESTER, (1R, 3S) -/CN
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 2-PHENYL-/CN
E6
             1
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 2-PHENYL-, DIMETHYL ESTER/C
E7
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 2-PHENYL-, POLYMER WITH 1,1
E8
             1
                   '-OXYBIS (4-ISOCYANATOBENZENE)/CN
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 2-PHENYL-, POLYMER WITH 1,4
E9
             1
                   -BENZENEDICARBOXYLIC ACID AND 1,1'-OXYBIS(4-ISOCYANATOBENZEN
                   E)/CN
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 4,5,6,7-TETRAFLUORO-2,3-DIH
E10
             1
                   YDRO-/CN
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 4-(ACETYLOXY)OCTAHYDRO-3A-M
E11
             1
                   ETHYL-6-(1-METHYLETHYL)-7-OXO-/CN
                   1H-INDENE-1,3-DICARBOXYLIC ACID, 5-FORMYL-, DIETHYL ESTER/CN
             1
E12
=>e3
             1 "1H-INDENE-1,3-DICARBOXYLIC ACID, 2,3-DIHYDRO-, CIS-"/CN
L1
=> d 11
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
L1
     69718-74-7 REGISTRY
RN
     Entered STN: 16 Nov 1984
ED
     1H-Indene-1,3-dicarboxylic acid, 2,3-dihydro-, cis- (9CI) (CA
CN
     INDEX NAME)
OTHER NAMES:
     cis-1,3-Indandicarboxylic acid
CN
     STEREOSEARCH
FS
     C11 H10 O4
MF
                  BEILSTEIN*, CA, CAPLUS, TOXCENTER
LC
     STN Files:
         (*File contains numerically searchable property data)
```

Relative stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> filke caplus

L2

0 FILKE 0 CAPLUS

0 FILKE CAPLUS

(FILKE (W) CAPLUS)

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 16.50 16.92

FULL ESTIMATED COST

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FILE COVERS 1907 - 22 Sep 2005 VOL 143 ISS 13 FILE LAST UPDATED: 21 Sep 2005 (20050921/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 11

L3 1 L1

=> d 13 ti fbib abs

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

TI Synthesis and pharmacological activity of 2,3,4,5-tetrahydro-1,5-methano-1H-3-benzazepines

AN 1979:432639 CAPLUS

DN 91:32639

TI Synthesis and pharmacological activity of 2,3,4,5-tetrahydro-1,5-methano-1H-3-benzazepines

AU Mazzocchi, Paul H.; Stahly, Barbara C.

CS Dep. Chem., Univ. Maryland, College Park, MD, USA

SO Journal of Medicinal Chemistry (1979), 22(4), 455-7 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CASREACT 91:32639

GΙ

The title compds. I (R = H, alkyl, allyl, etc.) were prepared from 2,3-dioxobenzonorbornene. 3-Allyl-2,3,4,5-tetrahydro-1,5-methano-1H-3-benzazepine oxalate (1:1) showed a slight antinociceptive activity in the mouse hot-plate assay and little antagonistic activity in the tail-flick assay. None of other I showed significant analgesic activity and all except 2,3,4,5-tetrahydro-3-(2-phenylethyl)-1,5-methano-1H-3-benzazepine oxalate (1:1) were toxic. Structure-activity relations are discussed.

=> logoff hold COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 4.45 21.37

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE -0.73 -0.73

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